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Willard L. Miranker

Numerical Methods for Stiff Equations

and Singular Perturbation Problems

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Editor's Preface

Approach your problems from the right end and begin with the answers. Then, one day, perhaps you will find the final question.
'The Hermit Clad in Crane Feathers' in R. Van Gulik's *The Chinese Maze Murders*.

It isn't that they can't see the solution. It is that they can't see the problem.

G. K. Chesterton, The scandal of Father Brown "The point of a pin"

Growing specialization and diversification have brought a host of monographs and textbooks on increasingly specialized topics. However, the 'tree' of knowledge of mathematics and related fields does not grow only by putting forth new branches. It also happens, quite often in fact, that branches which were thought to be completely disparate are suddenly seen to be related.

Further, the kind and level of sophistication of mathematics applied in various sciences has changed drastically in recent years: measure theory is used (non-trivially) in regional and theoretical economics; algebraic geometry interacts with physics; the Minkowsky lemma, coding theory and the structure of water meet one another in packing and covering theory; quantum fields, crystal defects and mathematical programming profit from homotopy theory; Lie algebras are relevant to filtering; and prediction and electrical engineering can use Stein spaces.

This series of books. *Mathematics and Its Applications*, is devoted to such (new) interrelations as *exempla gratia:*

- —a central concept which plays an important role in several different mathematical and/or scientific specialized areas;
- —new applications of the results and ideas from one area of scientific endeavor into another;
- —influences which the results, problems and concepts of one field of enquiry have and have had on the development of another.

With books on topics such as these, of moderate length and price, which are stimulating rather than definitive, intriguing rather than encyclopaedic, we hope to contribute something towards better communication among the practitioners in diversified fields.

The unreasonable effectiveness of mathematics in science . . .

Eugene Wigner

Well, if you knows of a better 'ole, go to it.

Bruce Bairnsfather

What is now proved was once only imagined.

William Blake

As long as algebra and geometry proceeded a long separate paths, their advance was slow and their applications limited.

But when these sciences joined company, they drew from each other fresh vitality and thenceforward marched on at a rapid pace towards perfection.

Joseph Louis Lagrange

Krimpen a/d IJssel
March, 1979.

MICHIEL HAZEWINKEL

Preface

Two principal approaches to the problems of applied mathematics are through numerical analysis and perturbation theory. In this monograph, we discuss and bring together a special body of techniques from each of these: (i) from numerical analysis, methods for stiff systems of differential equations, (ii) from perturbation theory, singular perturbation methods. Both of these areas are grounded in problems arising in applications from outside of mathematics for the most part. We cite and discuss many of them.

The mathematical problem treated is the initial value problem for a system of ordinary differential equations. However, results for other problems such as recurrences, boundary value problems and the initial value problem for partial differential equations are also included.

Although great advances have by now been made in numerical methods, there are many problems which seriously tax or defy them. Such problems need not be massive or ramified. Some are the simplest problems to state. They are those problems which possess solutions which are particularly sensitive to data changes or correspondingly problems for which small changes in the independent variable lead to large changes in the solution. These problems are variously called ill conditioned, unstable, nearly singular, etc. Stiff differential equations is a term given to describe such behavior for initial value problems.

Problems of this type have always attracted attention among mathematicians. The stiff differential equation is a relative late comer, its tardiness correlated perhaps to the development of powerful computers. However, in recent years a sizeable collection of results has emerged for this problem, although of course very much remains to be done. For example, the connection between stiff problems and other types of ill conditioned problems is easy to draw. However, there is a conspicuous paucity of methods of regularization, so commonly used for ill conditioned problems in the treatment of stiff equations.

Problems of singular perturbation type are also ill conditioned in the sense described here. These problems have been extensively and continuously studied for some time. Only relatively recently and also with the development of powerful computers has the numerical analysis of such problems begun in a significant way.

Of course the two problem classes overlap as do the sets of numerical methods for each. We include examples and applications as well as the results of illustrative computational experiments performed with the methods discussed here. We also see that these methods form the starting point for additional numerical study of other kinds of stiff and/or singularly perturbed problems. For this reason, numerical analyses of recurrences, of boundary value problems and of partial differential equations are also included.

Most of the material presented here is drawn from the recent literature. We refer to the survey of Bjurel, Dahlquist, Lindberg and Linde, 1972, to lecture notes of Liniger, 1974 and of Miranker, 1975, to three symposia proceedings, one edited by Willoughby, 1974, one by Hemker and Miller, 1979, and one by Axelsson, Frank and vander Sluis, 1980. These and citations made in the text itself to original sources are collected in the list of references. I cite particularly the work of F. C. Hoppensteadt to whom is due (jointly with myself) all of the multitime methodology which is presented here.

This monograph is an outgrowth of an earlier one which contained my lecture notes for courses given at the Université de Paris-Sud, (Orsay) and at the Instituto per le Applicazioni del Calcolo 'Mauro Picone', Rome during 1974–1975.

The presentation in this monograph reflects the current active state of the subject matter. It varies from formal to informal with many states in between. I believe that this shifting of form is not distracting, but on the contrary, it serves to stimulate understanding by exposing the applied nature of the subject on the one hand and the interesting mathematics on the other. It certainly shows the development of mathematics as a subject drawing on real problems and supplying them in turn with structure, a process of mutual enrichment. This so-called process of applied mathematics is one which I learned so many years ago as a student, first of E. Isaacson and then of J. B. Keller, and I do, with gratitude, dedicate this modest text to them.

I am grateful to R. A. Toupin, the Director of the Mathematical Sciences

Department of the IBM Research Center for his interest in and for his support of this work. For the physical preparation of the text, I must thank Jo Genzano, without whose help I would not have dared to attempt it.

Yorktown Heights, 1979 W. L. M.

Table of Contents

Chapter 1

Introduction

Summary

In the first section of this chapter, we introduce the problem classes to be studied in this monograph. In the second section, we review the classical linear multistep theory for the numerical approach to ordinary differential equations.

The problem classes, which as we will see are rather closely related to each other, are stiff differential equations and differential equations of singular perturbation type. Our introduction to them is complemented by the presentation examples both of model problems and of actual applications.

These two problem classes seriously defy traditional numerical methods. The numerical approach to these problems consists of exposing the limitations of the traditional methods and the development of remedies. Thus, we include the review of the linear multistep theory here since it is the traditional numerical theory for differential equations and as such it supplies the point of departure of our subject.

1.1. STIFFNESS AND SINGULAR PERTURBATIONS

1.1.1. *Motivation*

Stiff differential equations are equations which are *ill-conditioned* in a computational sense. To reveal the nature of the ill-conditioning and to motivate the need to study numerical methods for stiff differential equations, let us consider an elementary error analysis for the *initial value problem*

$$\begin{aligned} \dot{y} &= -Ay, \qquad 0 < t \le \bar{t}, \\ y(0) &= y_0. \end{aligned} \tag{1.1.1}$$

Here y is an m-vector and A is a constant $m \times m$ matrix. The dot denotes time differentiation. Corresponding to the increment $h > 0$, we introduce the *mesh points* $t_n = nh$, $n = 0, 1, \ldots$. The solution

$$\boldsymbol{y}_n = \boldsymbol{y}(t_n),$$

of (1.1.1) obeys the recurrence relation,

$$\boldsymbol{y}_{n+1} = \mathrm{e}^{-Ah}\boldsymbol{y}_n. \tag{1.1.2}$$

For convenience we introduce the function $S(z) = \mathrm{e}^{-z}$, and we rewrite (1.1.2) as

$$\boldsymbol{y}_{n+1} = S(Ah)\boldsymbol{y}_n. \tag{1.1.3}$$

The simplest numerical procedure for determining an approximation $\boldsymbol{u}_n$ to $\boldsymbol{y}_n$, $n = 1, 2, \ldots$, is furnished by *Euler's method*,

$$\begin{aligned} \boldsymbol{u}_{n+1} - \boldsymbol{u}_n &= -hA\boldsymbol{u}_n, \qquad n = 1, 2, \ldots, \\ \boldsymbol{u}_0 &= \boldsymbol{y}_0. \end{aligned} \tag{1.1.4}$$

Using the function $K(z) = 1 - z$, we may rewrite (1.1.4) as

$$\boldsymbol{u}_{n+1} = K(Ah)\boldsymbol{u}_n. \tag{1.1.5}$$

$K(z)$ is called the *amplification factor* and $K(Ah)$ the *amplification operator* corresponding to the difference equation (1.1.4).

By subtracting (1.1.5) from (1.1.3), we find that the *global error*,

$$\boldsymbol{e}_n = \boldsymbol{u}_n - \boldsymbol{y}_n,$$

obeys the recurrence relation

$$\boldsymbol{e}_{n+1} = K\boldsymbol{e}_n + T\boldsymbol{y}_n. \tag{1.1.6}$$

Here $T = K - S$ is the *truncation operator*. (1.1.6) may be solved to yield

$$\boldsymbol{e}_{n+1} = \sum_{j=0}^{n} K^j T\boldsymbol{y}_{n-j},$$

from which we obtain the bound

$$\|\boldsymbol{e}_n\| \le n \max_{0 \le j \le n-1} \|K\|^j \max_{0 \le j \le n-1} \|T\boldsymbol{y}_j\|. \tag{1.1.7}$$

Note that $nh \le \bar{t}$. Here and throughout this text (and unless otherwise specified) the double bars, $\|\cdot\|$, denote some vector norm or the associated matrix norm, as the case may be.

If the numerical method is *stable*, *i.e.*,

$$\| K \| \le 1 \tag{1.1.8}$$

and *accurate* of *order* *p*, *i.e.*,

$$\| Ty \| = O(h^{p+1}) \| y \|, \tag{1.1.9}$$

then the bound (1.1.7) shows that $\| e_n \| = O(h^p)$. (Of course for Euler's method, to which case we restrict ourselves, $p = 1$.)

To demonstrate (1.1.9), we note that $\| y \|$ is bounded as a function of t for $0 \le t \le \bar{t}$, and we show that $\| T \| = O(h^2)$. For the latter we use the *spectral representation theorem* which contains the assertion

$$T(hA) = \sum_{j=1}^{m} T(h\lambda_j) P_j(A). \tag{1.1.10}$$

Here we assume that the eigenvalues $\lambda_j, j = 1, \ldots, m$ of A are distinct. The $P_j(z)$, $j = 1, \ldots, m$ are the *fundamental polynomials* on the spectrum of A. (i.e., $P_j(z)$ is the polynomial of minimal degree such that $P_j(\lambda_i) = \delta_{ij}$, $i, j = 1, \ldots, m$. Here δ_{ij} is the Kronecker delta.)

We have chosen $T(z) = K(z) - S(z)$ to be small at a single point, $z = 0$. Indeed

$$T(z) = O(z^2).$$

This and (1.1.10) assures that $\| T \| = O(h^2)$. More precisely we have that

$$\| T \| = O(|\lambda_{\max}|^2 h^2), \tag{1.1.11}$$

where

$$|\lambda_{\max}| = \max_{1 \le j \le m} |\lambda_j|.$$

One proceeds similarly, using the spectral representation theorem to deal with the requirement of stability. For Euler's method we obtain stability if

$$|1 - h\lambda_j| \le 1, \qquad j = 1, \ldots, m. \tag{1.1.12}$$

(See Definition 1.2.11 and Theorem 1.2.12 below.)

For the usual equations encountered in numerical analysis, $|\lambda_{\max}|$ is not too large, and (1.1.12) is achieved with a reasonable restriction on the size of h. In turn (1.1.11) combined with the bound (1.1.7) for $\| e_n \|$ yields an acceptable error size for a reasonable restriction on the size of h.

1.1.2. *Stiffness*

For the time being at least, *stiffness* will be an informal idea.

A *stiff system* of equations is one for which $|\lambda_{max}|$ is enormous, so that either the stability or the error bound or both can only be assured by unreasonable restrictions on h (i.e., an excessively small h requiring too many steps to solve the initial value problem). Enormous means, enormous relative to a scale which here is $1/\bar{t}$. Thus, an equation with $|\lambda_{max}|$ small may also be viewed as stiff if we must solve it for great values of time.

In the literature, stiffness for the system (1.1.1) of differential equations is frequently found to be defined as the case where the ratio of the eigenvalues of A of largest and smallest magnitude, respectively, is large. This definition is unduly restrictive. Indeed as we may see, a single equation can be stiff. Moreover, this usual definition excludes the obviously stiff system corresponding to a high frequency harmonic oscillator, viz.

$$\ddot{y} + \omega^2 y = 0, \qquad \omega^2 \text{ large}. \tag{1.1.13}$$

Indeed neither definition is entirely useful in the nonautonomous or nonlinear case. While stiffness is an informal notion, we can include most of the problems which are of interest by using the idea of *ill-conditioning* (i.e., *instability*). Suppose we develop the numerical approximation to the solution of a differential equation along the points of a mesh, for example, by means of a relation of the type (1.1.5). If small changes in $\boldsymbol{u}_n$ in (1.1.5) result in large changes in $\boldsymbol{u}_{n+1}$, then the numerical method represented by (1.1.5), when applied to the problem in question, is ill-conditioned. To exclude the case wherein this unstable behavior is caused by the numerical method and is not a difficulty intrinsic to the differential equations, we will say that a system of differential equations is stiff if this unstable behavior occurs in the solutions of the differential equations. More formally we have the following definition.

DEFINITION 1.1.1. A system of differential equations is said to be stiff on the interval $[0, \bar{t}]$, if there exists a solution of that system a component of which has a variation on that interval which is large compared to $1/\bar{t}$.

We make the following observation about the informal nature of our discussion.

REMARK 1.1.2. We may ask what the term 'large compared to' signifies in a formal definition. In fact it has no precise meaning, and we are allowing informal notions (like: reasonable restriction, enormous, acceptable, too many, etc.) with which some numerical analysts feel comfortable to find their way into a formal mathematical statement. While allowing this risks some confusion, we will for reasons of convenience continue to do so. In order to minimize this risk and as a model for similar questions, we now explain how this informality could be repaired in the context of Definition 1.1.1. Hereafter we will not return to this point for other similar problems. The repair is made by replacing single objects by a class of objects out of which the single object is drawn.

For example, a proper alternate to Definition 1.1.1 could be the following.

DEFINITION 1.1.3. A collection of systems of differential equations is said to be stiff on an interval $[0,\bar{t}]$, if there exists no positive constant M such that the variation of every component of every solution of every member of the collection is bounded by M.

The following example shows how treacherous the reliance on eigenvalues to characterize stiffness can be; even in the linear case.

Example

$$\dot{y} = A(t)y, \tag{1.1.14}$$

where

$$A(t) = \begin{bmatrix} \sin \omega t & \cos \omega t \\ \cos \omega t & -\sin \omega t \end{bmatrix}.$$

The eigenvalues of $A(t)$ are ± 1. The matrizant of (1.1.14) is

$$\Phi(t) = B(t)\frac{\sinh \sigma}{\sigma} + I \cosh \sigma.$$

Here I is the 2×2 identity matrix,

$$\sigma = \sqrt{2}(1 - \cos \omega t)^{1/2}$$

and

$$B(t) = \frac{1}{\omega}\begin{bmatrix} 1 - \cos \omega t & \sin \omega t \\ \sin \omega t & \cos \omega t - 1 \end{bmatrix}.$$

Thus for $\omega \to \infty$,

$$\Phi(t) = (\cosh\sqrt{2 - 2\cos \omega t})(1 + O(\omega^{-1}))I$$

uniformly for $t \in [0,\bar{t}]$.